

Supporting Information

Fluorenylethynylpyrene Derivatives with Strong Two-Photon Absorption: Influence of Substituents on Optical Properties

C. Lavanya Devi,^{a,b} K. Yesudas,^b Nikolay S. Makarov,^{c,d} V. Jayathirtha Rao^{*,a,e} K. Bhanuprakash^{*,b,e} and Joseph W. Perry^{*c}

^a*Crop Protection Chemicals Division, ^bInorganic and Physical Chemistry Division, ^cAcSIR, CSIR-Indian Institute of Chemical Technology, Uppal Road, Tarnaka, Hyderabad - 500 007, India.*

^c*School of Chemistry and Biochemistry and Center for Organic Photonics and Electronics, Georgia Institute of Technology, Atlanta, Georgia 30332-0400, United States.*

^d*Currently at Center for Advanced Solar Photophysics, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, United States.*

Corresponding Author: jrao@iict.res.in

Figure S1: Normalized absorption spectra of all the compounds in different solvents measured at 1.0×10^{-6} M concentration.

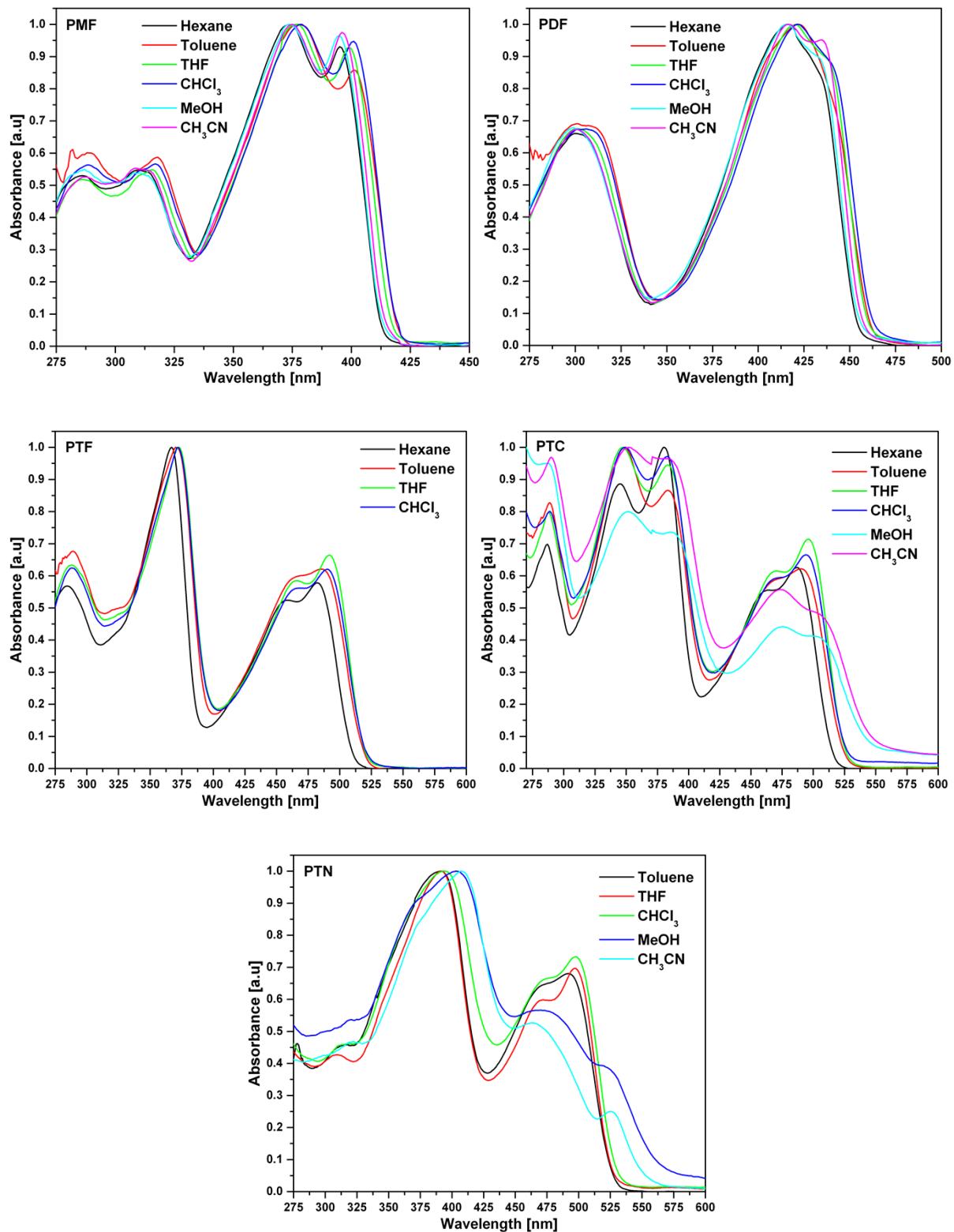


Figure S2: Concentration dependent absorption spectra of compounds **PTC** and **PTN** in CH₃CN and CH₃OH measured at 1.0×10⁻⁶ to 1.0×10⁻⁵ M concentration.

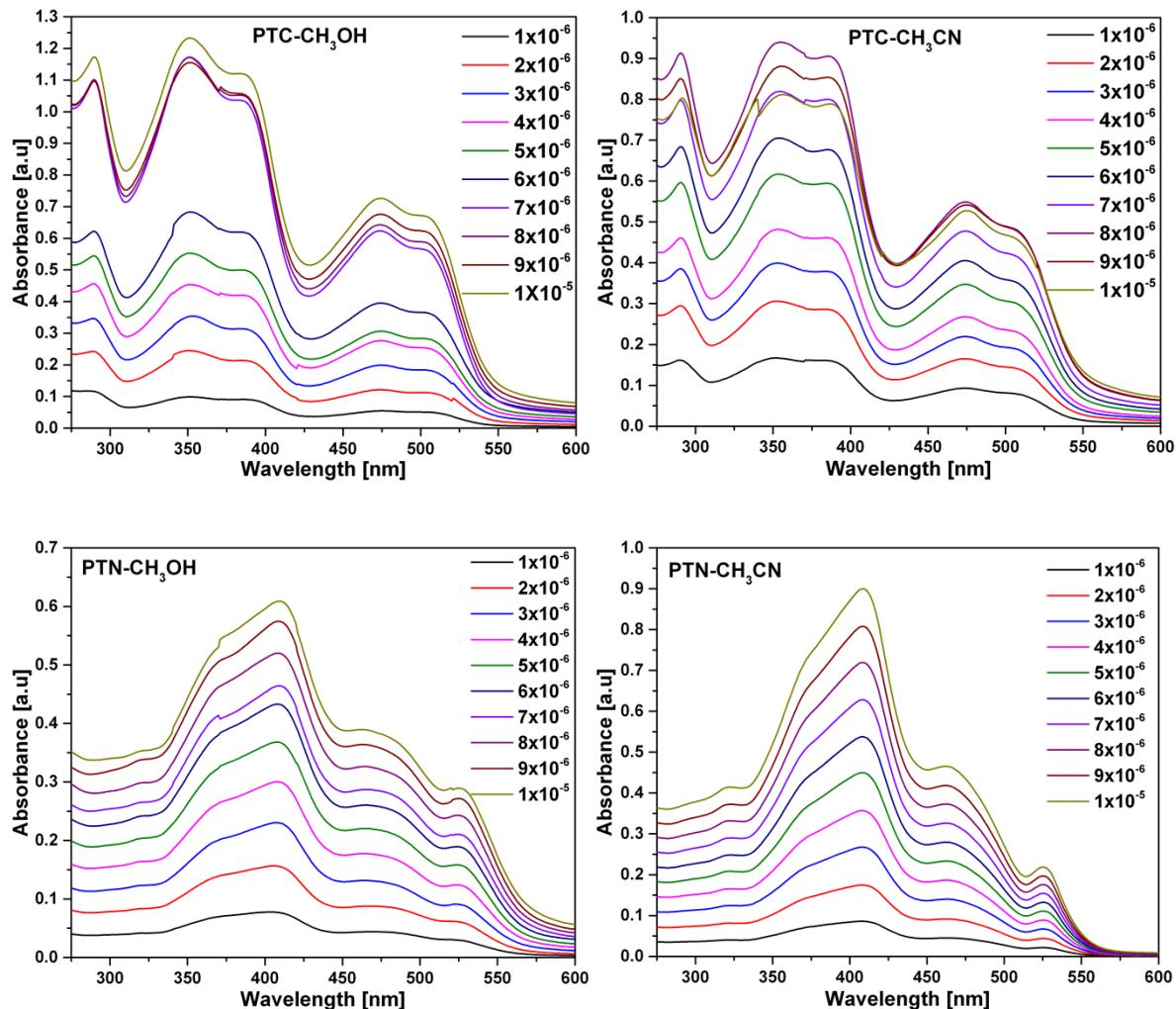


Figure S3. Solvatochromic shifts of the absorption (a) and emission (b) of all the compounds measured in solvents with varied polarity.

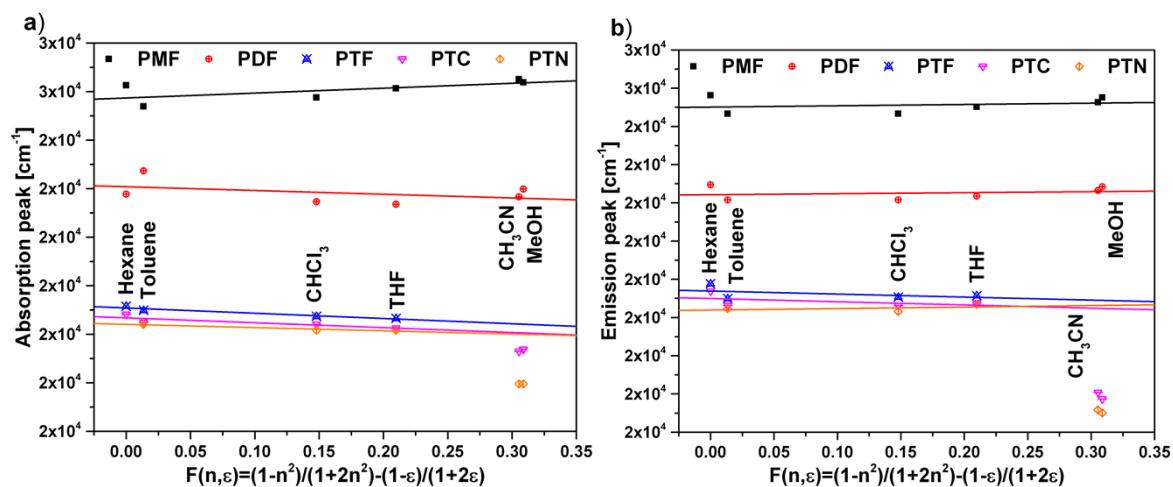


Figure S4: Normalized fluorescence spectra of all the compounds in different solvents measured at 1.0×10^{-6} M concentration, excited at their corresponding maximum wavelengths.

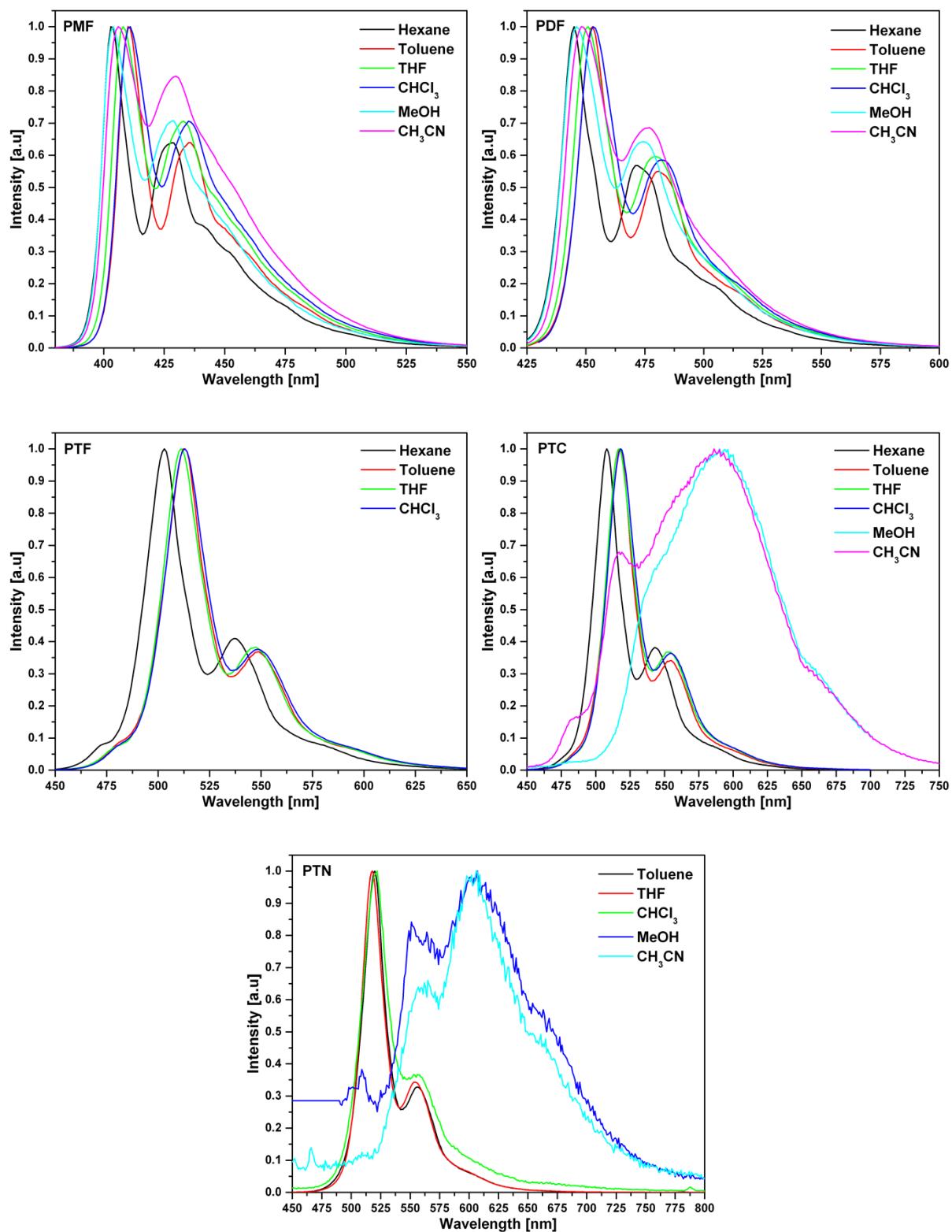


Table S1: Absorption wavelengths (λ_{max} , nm), molar extinction coefficient (ϵ , $M^{-1}cm^{-1}$), emission wavelengths (λ_{emi} , nm) and quantum yield (Φ) of all the compounds measured in different solvents.

Compound	Solvent	$\lambda_{\text{max}} (\epsilon, M^{-1} Cm^{-1})^a$	λ_{emi}^b	Φ^c
PMF	Hexane	398(67040), 369(73540), 315(40770), 283(40280)	403, 428	0.97
	Toluene	405(58200), 375(67900), 318(40100), 288(41100)	411, 436	0.95
	THF	399(67880), 376(73400), 315(40220), 285(38010)	408, 433	0.89
	CHCl ₃	402 (65950), 378 (70180), 315(39310), 286(39010)	411, 436	0.97
	MeOH	397(41900), 374(44730), 314(23690), 283(24040)	404, 429	0.96
	CH ₃ CN	396(69880), 374(71540), 312(39310), 285(37310)	406, 429	0.91
PDF	Hexane	437(88090), 414(111390), 301(73790)	445, 471	0.94
	Toluene	428(98900), 303(67900)	453, 480	0.98
	THF	441(99470), 421(116970), 300(78940)	451, 480	0.98
	CHCl ₃	440(87690), 423(99610), 305(0.06722)	453, 482	0.99
	MeOH	435(93680), 415(106350), 301(71690)	446, 474	0.95
	CH ₃ CN	438(97530), 411(102530), 300(71310)	448, 476	0.81
PTF	Hexane	486(97020), 453(88330), 367(172460), 284(97910)	503,537	0.57
	Toluene	488(80900), 462(79100), 371(134000), 289(90300)	513,548	0.59
	THF	492(92610), 462(80560), 373(139460), 286(88070)	511,547	0.53
	CHCl ₃	491(93360), 464(84220), 372(150730), 288(94060)	512, 549	0.48
PTC	Hexane	490(106880), 458(94640), 380(173970), 344(153980)	508,543	0.44
	Toluene	494(99700), 467(94600), 385(140000), 348(162000)	518,554	0.56
	THF	497(120790), 465(102320), 383(160170), 347(169480)	516,552	0.53
	CHCl ₃	495(105090), 468(93220), 382(153400), 350(158010)	518, 555	0.47
	MeOH	508(49470), 473(54350), 390(89920), 350(98650)	593	0.11
	CH ₃ CN	509(77870), 476(92750), 390(157260), 348(165670)	483,517,587	0.12
PTN	Toluene	495(77100), 468(72600), 391(114000), 311(52000)	520,556	0.55

THF	498(82800), 471(71010), 391(118790), 311(50600)	517,554	0.51
CHCl ₃	498(85640, 470(76540), 394(116840), 314(53610)	522,557	0.02
MeOH	527(28960), 480(43280), 407(77320), 371(70210)	553,606	0.001
CH ₃ CN	527(21370), 472(43860), 410(85670), 319(40130)	560,603	0.005

^a λ_{max} of the 1PA spectra in nm measured at 5.0×10^{-6} M concentration (values in parenthesis corresponds to the molar extinction coefficients).

^b λ_{max} of the one-photon fluorescence spectra in nm measured at 1.0×10^{-6} M concentration.

^cFluorescence quantum yield measured by taking diphenylanthracene (0.9Φ in cyclohexane) as standard with a deviation of $\pm 10\%$.

Table S2: Absorption and emission solvatochromic slopes (cm^{-1}) of all the compounds measured in different solvents.

Compound	Absorption slope ^a	Emission slope ^a
PMF	1009	345
PDF	-771	260
PTF	-1081	-788
PTC	-1008	-838
PTN	-666	844

^aAcetonitrile and methanol points are excluded for **PTC** and **PTN**.